8. DATA INTERPOLATION AND EXTRAPOLATION EFFECTS

As explained in Section 5.1., QTRACER utilizes a very efficient data interpolation routine. The primary use of the data interpolation routine would be if the user believes that missing datapoints can be reasonably approximated by data interpolation. For example, if the user believes that unaltered tracer-breakthrough curves suggest that data aliasing may have occurred, then data interpolation may be able to confirm or deny if aliasing really has occurred.

8.1. COMPARISON OF ATKIN.DAT OUTPUT FILES

To illustrate the effect of data interpolation, data extrapolation, and the combined effect of data interpolation and extrapolation on a data set exhibiting good mass recovery, the ATKIN.DAT data set was subjected to each of these three algorithms. In some instances, the effect is fairly noticeable while in other instances there are no differences.

8.1.1. Interpolated ATKIN.DAT Tracer-Breakthrough Curve

Figure 28 depicts the interpolated tracer-breakthrough curve generated by QTRACER and analyzed by QTRACER. Note that discharge has an interpolated value for each time an interpolated tracer concentration value was created.

Graphically, the user will note that Figure 28 is more reasonable than Figure 16. The improvement is most evident at the peak, where the interpolated file more correctly matches the peak concentration datapoint. In Figure 16, the peak concentration is actually exceeded by the graphics line. However, the apparent inaccurate plotting is *NOT* reflected in the actual data analysis by QTRACER.

8.1.2. Interpolated ATKIN.DAT Chatwin Plot

Figure 29 depicts the interpolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the equation for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER.

Some difference will be noted between Figure 29 and Figure 17, but not a significant difference. Interpolation results in more datapoints falling on the necessary straight line and the equation of the straight line has different values for the y intercept and slope. As such, a slightly different estimate for longitudinal dispersion will result.

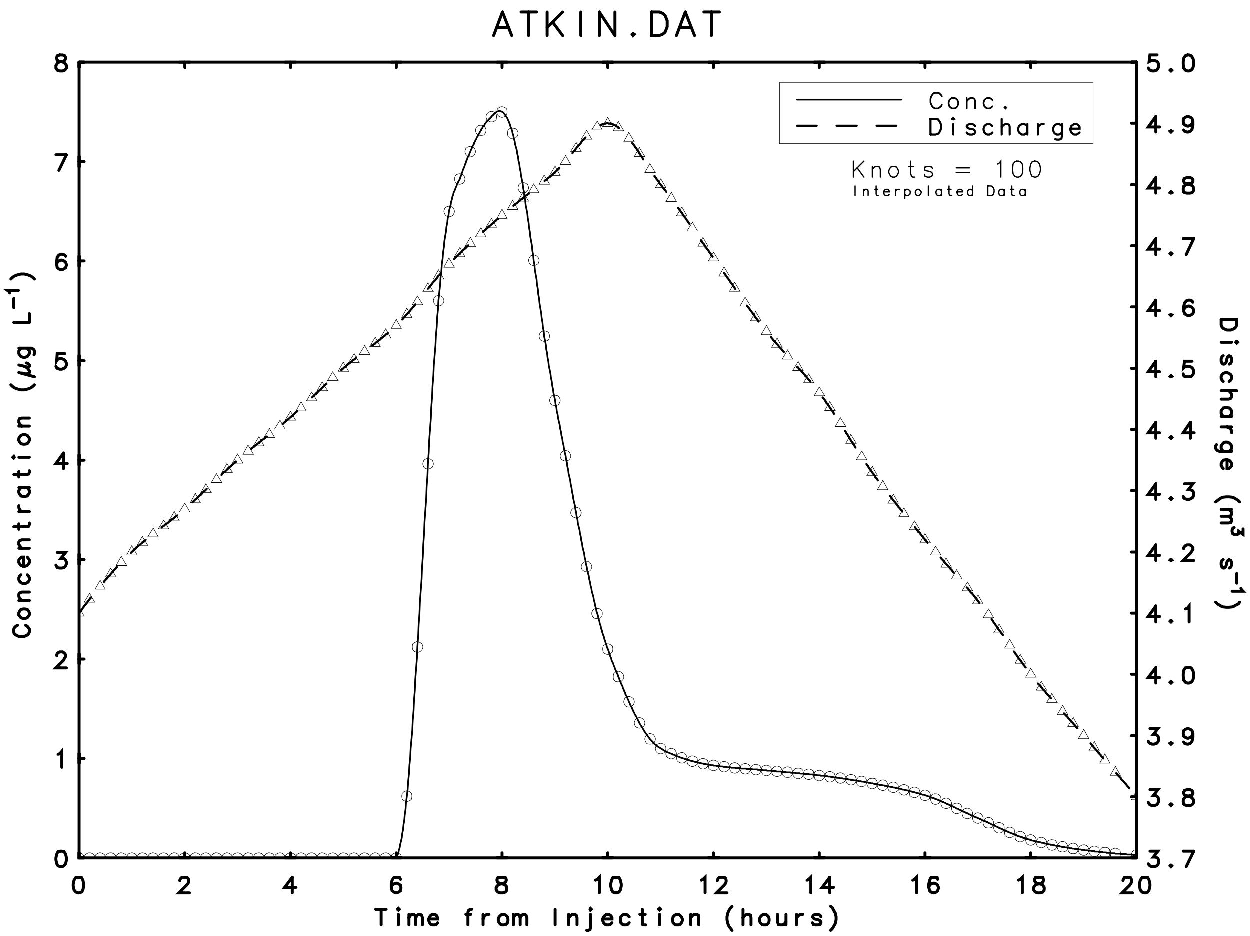

Figure 28. Interpolated curve for the ATKIN.DAT sampling station data file.

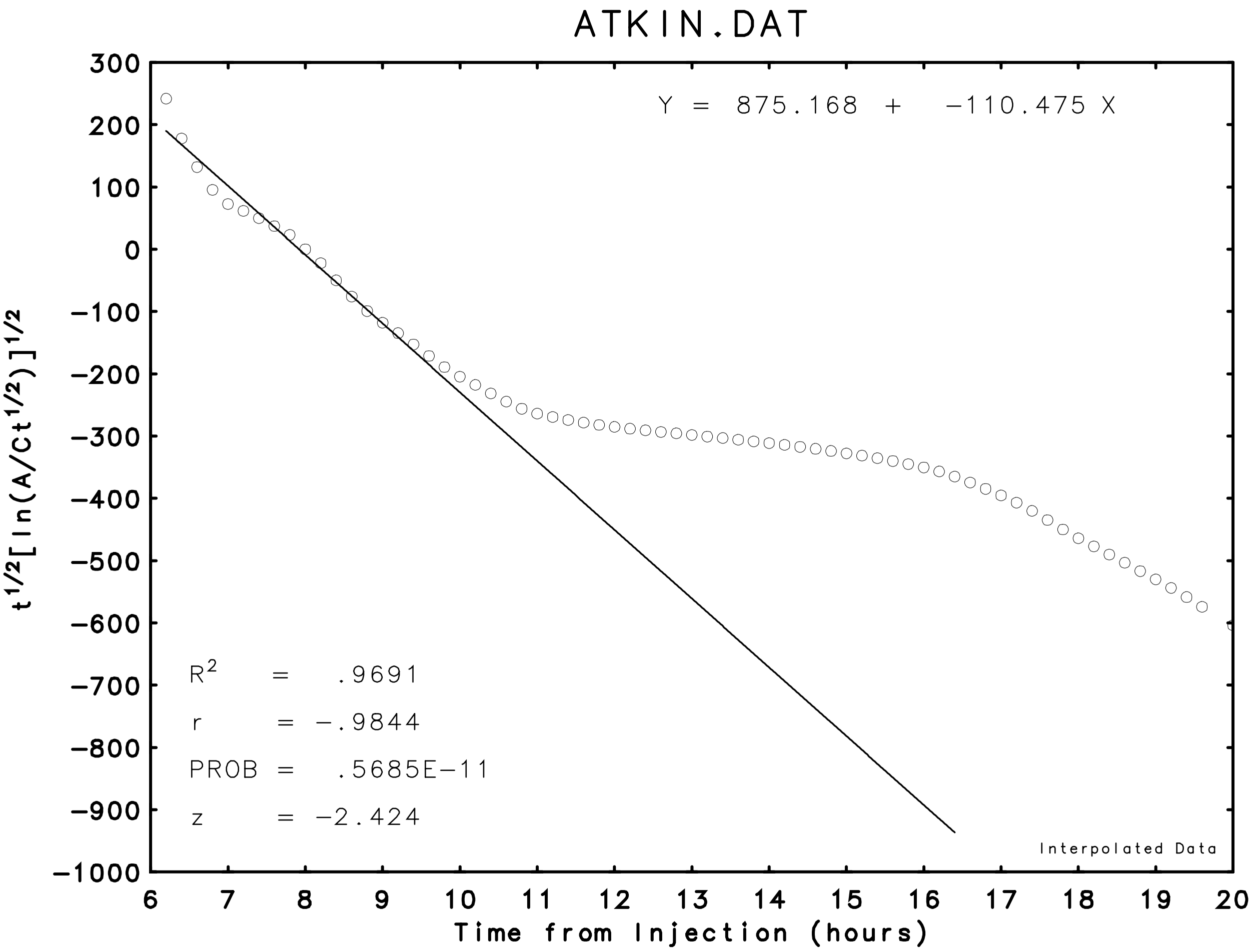

Figure 29. Interpolated data set for the Chatwin parameter for the ATKIN.DAT sampling station data file.

Table 6 compares the final analytical output for the unaltered tracer-breakthrough curve for the ATKIN.DAT data set, the interpolated ATKIN.DAT data set, and the Interpolated-extrapolated ATKIN.DAT data set. Note how each file's results are closely matched with the others.

8.1.3. Extrapolated ATKIN.DAT Tracer-Breakthrough Curve

Figure 30 depicts the extrapolated tracer-breakthrough curve generated and analyzed by QTRACER. Note that discharge has an interpolated value for each time an extrapolated tracer concentration value was created.

Graphically, the user will note that the tracer-breakthrough curve shown in Figure 30 appears relatively unchanged from Figure 16. The only apparent difference is that the elapsed tracer travel time has been extended from 20 hours to > 22 hours and that one additional datapoint (total data $= 22$) has been included.

More obvious is the effect of data extrapolation on the discharge curve when data extrapolation routines `1` (exponential decay) and `3` (statistical fit) are employed (`3` = statistical fit for Figure 30). Extrapolation routine `2` (piecewise cubic Hermite) uses the shape of the entire existing data curve to determine the "most reasonable" extrapolation datapoint possible for the extrapolated discharge.

Extrapolation routines `1` and `3`, however, have no mathematical basis for consideration. For example, there is no reason to assume that discharge will behave as an exponential decay function, so extrapolation routine `1 = exponential decay` would make no physical sense. Therefore, when extrapolation routines `1` or `3` are requested and a variable discharge was measured, QTRACER will automatically extend the discharge curve in the opposite vertical direction (along the y axis) to one-half its previous range. It is up to the user to decide on its reasonableness.

8.1.4. Extrapolated ATKIN.DAT Chatwin Plot

Figure 31 depicts the extrapolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the straight-line fit, the equation for the straight-line, and the relevant statistics describing the straight-line fit generated by QTRACER are identical to Figure 17. Data extrapolation had no effect on the Chatwin method analysis because original sample had resulted in nearly "complete" tracer recovery.

Table 6. Estimated hydraulic flow and geometric parameters from tracer-breakthrough curves for ATKIN.DAT sampling station.

Parameter	ATKIN.DAT (unaltered)	ATKIN.DAT (interpolated)	ATKIN.DAT[1] (extrapolated)	ATKIN.DAT[2] (inter./extra.)
Tracer Mass Recovered, g	4.48×10^{2}	4.48×10^{2}	4.48×10^{2}	4.48×10^{2}
Percent Mass Recovered	9.96×10^{1}	9.95×10^{1}	9.96×10^{1}	9.96×10^{1}
Accuracy Index	4.48×10^{-3}	4.75×10^{-3}	3.67×10^{-3}	3.80×10^{-3}
Initial Tracer Breakthrough, h	7.00×10^{0}	6.20×10^{0}	7.00×10^{0}	6.10×10^{0}
Time to Peak Concentration, h	8.00×10^{0}	8.00×10^{0}	8.00×10^{0}	8.00×10^{0}
Mean Tracer Residence Time, h	9.27×10^{0}	9.26×10^{0}	9.28×10^{0}	9.27×10^{0}
Elapsed Tracer Travel Time, h	2.00×10^{1}	2.00×10^{1}	2.26×10^{1}	2.32×10^{1}
Maximum Tracer Flow Velocity, m s^{-1}	1.07×10^{-1}	1.21×10^{-1}	1.07×10^{-1}	1.23×10^{-1}
Peak Tracer Flow Velocity, m s^{-1}	9.38×10^{-2}	9.38×10^{-2}	9.38×10^{-2}	9.38×10^{-2}
Mean Tracer Flow Velocity, m s^{-1}	8.09×10^{-2}	8.10×10^{-2}	8.08×10^{-2}	8.09×10^{-2}
Shear Velocity, m s^{-1}	1.70×10^{-2}	1.70×10^{-2}	1.70×10^{-2}	1.70×10^{-2}
Longitudinal Dispersion, m^2 s^{-1}	3.26×10^{0}	2.38×10^{0}	3.26×10^{0}	2.13×10^{0}
Hydraulic Head Loss, m	1.20×10^{-2}	1.21×10^{-2}	1.20×10^{-2}	1.20×10^{-2}

Listed parameters without dimensions are dimensionless.
[1]Extrapolated using a statistical straight line fit.
[2]Extrapolated using a cubic Hermite function.

Table 6. Estimated hydraulic flow and geometric parameters from tracer-breakthrough curves for ATKIN.DAT sampling station (cont.).

Parameter	ATKIN.DAT (unaltered)	ATKIN.DAT (interpolated)	ATKIN.DAT[1] (extrapolated)	ATKIN.DAT[2] (inter./extra.)
Conduit Volume, m^3	1.49×10^5	1.49×10^5	1.50×10^3	1.50×10^3
Conduit Cross-Sectional Area, m^2	5.53×10^1	5.53×10^1	5.54×10^1	5.54×10^1
Conduit Surface Area, m^2	5.16×10^7	5.16×10^7	5.15×10^7	5.15×10^7
Tracer Sorption Coefficient, m	1.31×10^{-5}	1.38×10^{-5}	1.07×10^{-5}	1.11×10^{-5}
Conduit Diameter, m	8.39×10^0	8.40×10^0	8.40×10^0	8.40×10^0
Hydraulic Depth, m	6.59×10^0	6.59×10^0	6.60×10^0	6.59×10^0
Friction Factor	1.12×10^{-1}	1.12×10^{-1}	1.12×10^{-1}	1.12×10^{-1}
Laminar Flow Sublayer, m	1.38×10^{-3}	1.38×10^{-3}	1.38×10^{-3}	1.38×10^{-3}
Reynolds Number	5.96×10^5	5.96×10^5	5.95×10^5	5.96×10^5
Froude Number	1.01×10^{-2}	1.01×10^{-2}	1.01×10^{-2}	1.01×10^{-2}
Peclet Number	7.77×10^1	1.06×10^2	7.77×10^1	1.19×10^2
Schmidt Number	1.14×10^3	1.14×10^3	1.14×10^3	1.14×10^3
Sherwood Number	1.49×10^4	1.49×10^4	1.49×10^4	1.49×10^4
Mass Transfer Coefficient, m s^{-1}	1.78×10^{-6}	1.78×10^{-6}	1.78×10^{-6}	1.78×10^{-2}
Molecular diffusion layer, m	5.62×10^{-4}	5.62×10^{-4}	5.62×10^{-4}	5.63×10^{-4}

Listed parameters without dimensions are dimensionless.
[1]Extrapolated using a statistical straight line fit.
[2]Extrapolated using a cubic Hermite function.

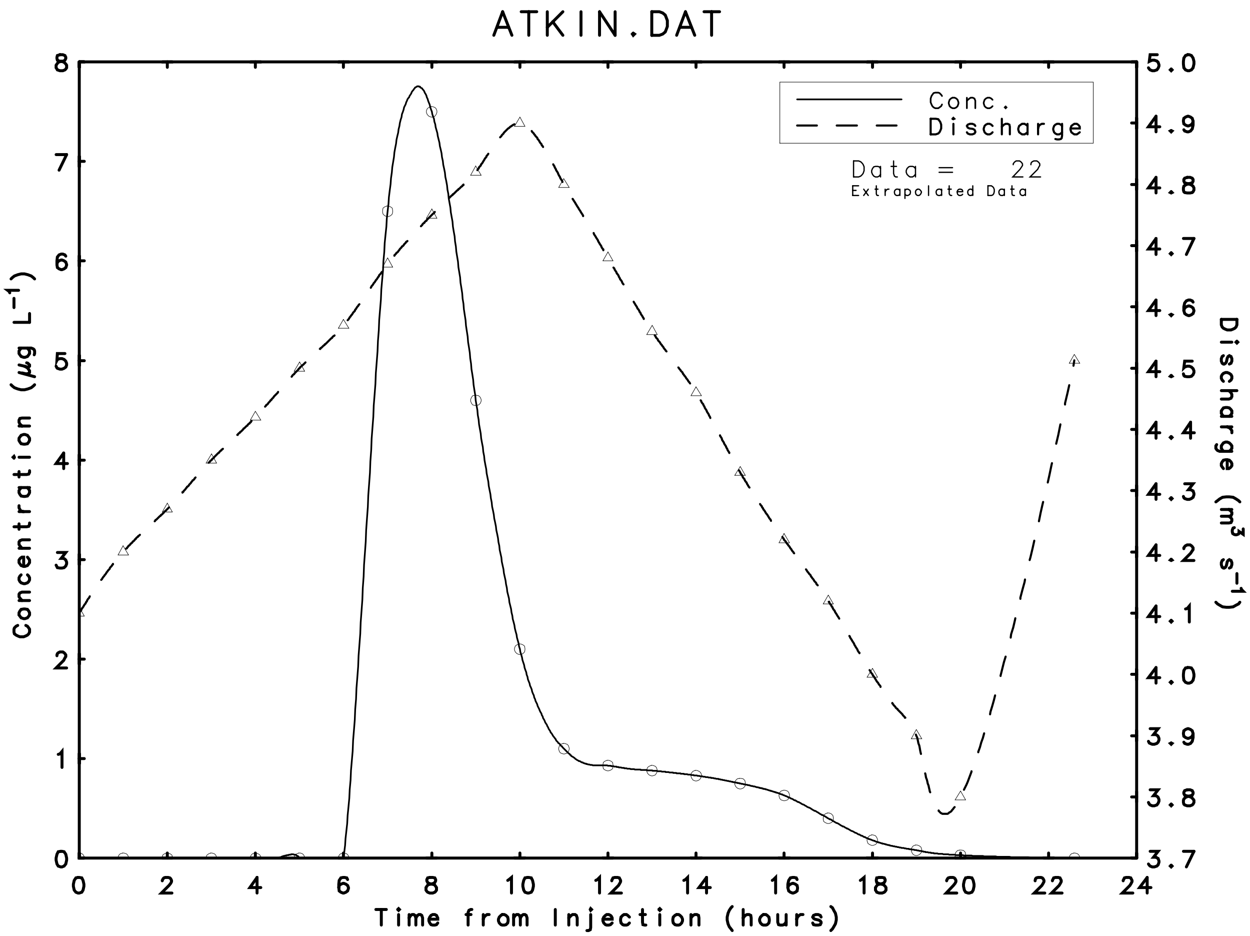

Figure 30. Extrapolated curve for the ATKIN.DAT sampling station data file.

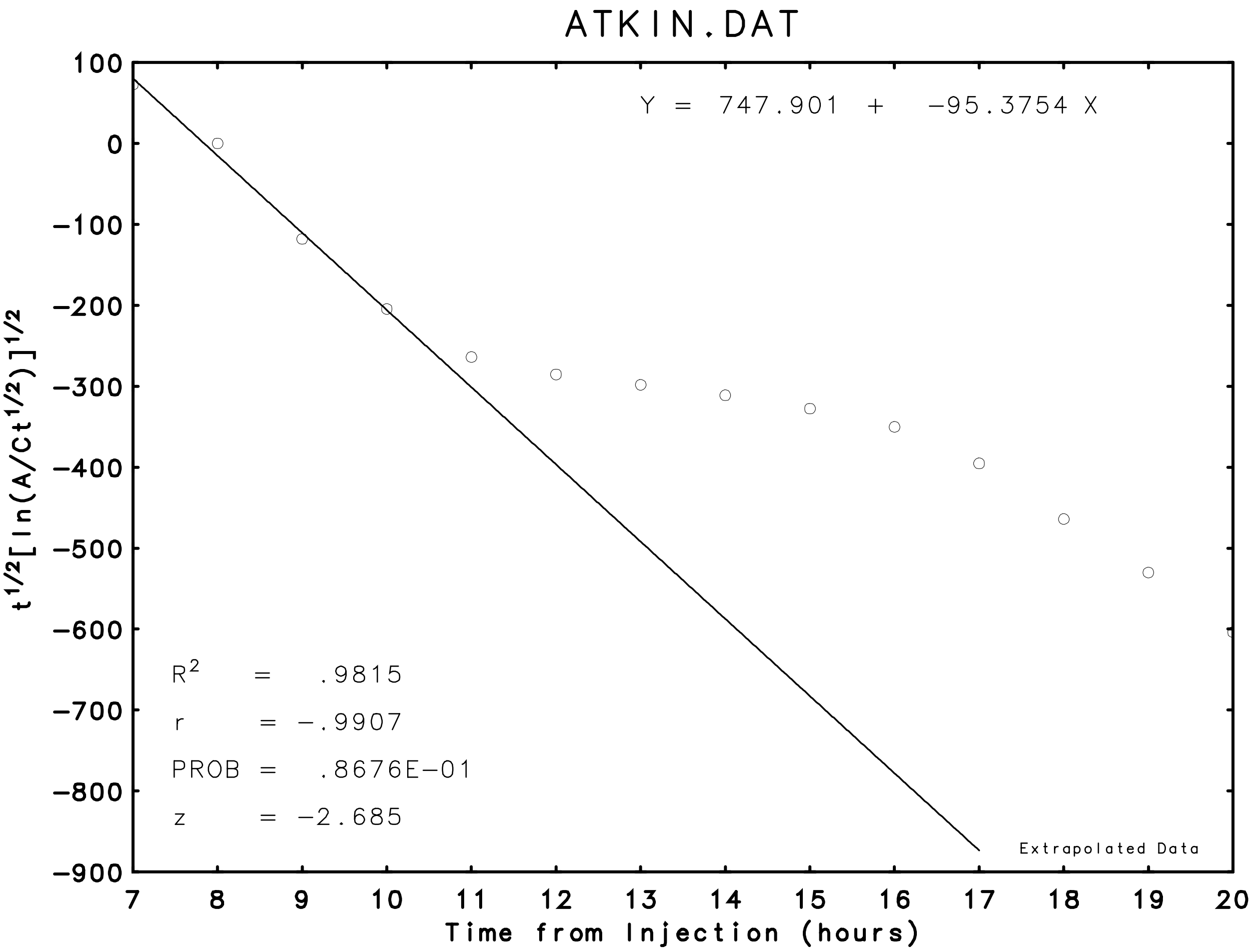

Figure 31. Extrapolated data set for the Chatwin parameter for the ATKIN.DAT sampling station data file.

8.2. INTERPOLATED-EXTRAPOLATED ATKIN.DAT DATA

Figures 32 and 33 illustrates how the interpolation and extrapolation routines provided in QTRACER can be used to in tracer-breakthrough curve analyses. Table 6 illustrates that there are no significant differences in any of the analyses provided by QTRACER for the ATKIN.DAT data set.

A more erratic tracer-breakthrough curve, or one that was ended leaving a significant mass of tracer in the system, would result in large differences when data interpolation and/or extrapolation is employed. The user should note that when data extrapolation is employed without data interpolation, the graphics may appear incorrect (*i.e.*, a straight-line connection from the last measured datapoint to the extrapolated datapoint). This apparent inaccuracy is not a problem, however, as it is strictly an artifact of the plotting algorithm. The integration routine used by QTRACER will develop a smooth curve between all provided datapoints regardless of tracer-breakthrough curve appearance.

8.3. COMPARISON OF RCA.DAT OUTPUT FILES

To further illustrate the effect of data interpolation, data extrapolation, and the combined effects of data interpolation and extrapolation on a data set exhibiting poor mass recovery, the RCA.DAT data set was subjected to each of these three algorithms. In some instances, the effect is fairly noticeable, while in other instances there are no differences.

8.3.1. Interpolated RCA.DAT Tracer-Breakthrough Curve

Figure 34 depicts the interpolated tracer-breakthrough curve generated and analyzed by QTRACER. Note that discharge has no interpolated value. This is because discharge was considered a constant, so there are no data to interpolate.

Graphically, the user will note that Figure 34 is little changed from the curve shown in Figure 22. The slight improvement is most evident at the peak, where the interpolated file more correctly matches the peak concentration datapoint. In Figure 22, the graphics line slightly exceeds the time to peak concentration. However, the apparent inaccurate plotting is *NOT* reflected in the actual data analysis by QTRACER.

8.3.2. Interpolated RCA.DAT Chatwin Plot

Figure 35 depicts the interpolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the equation

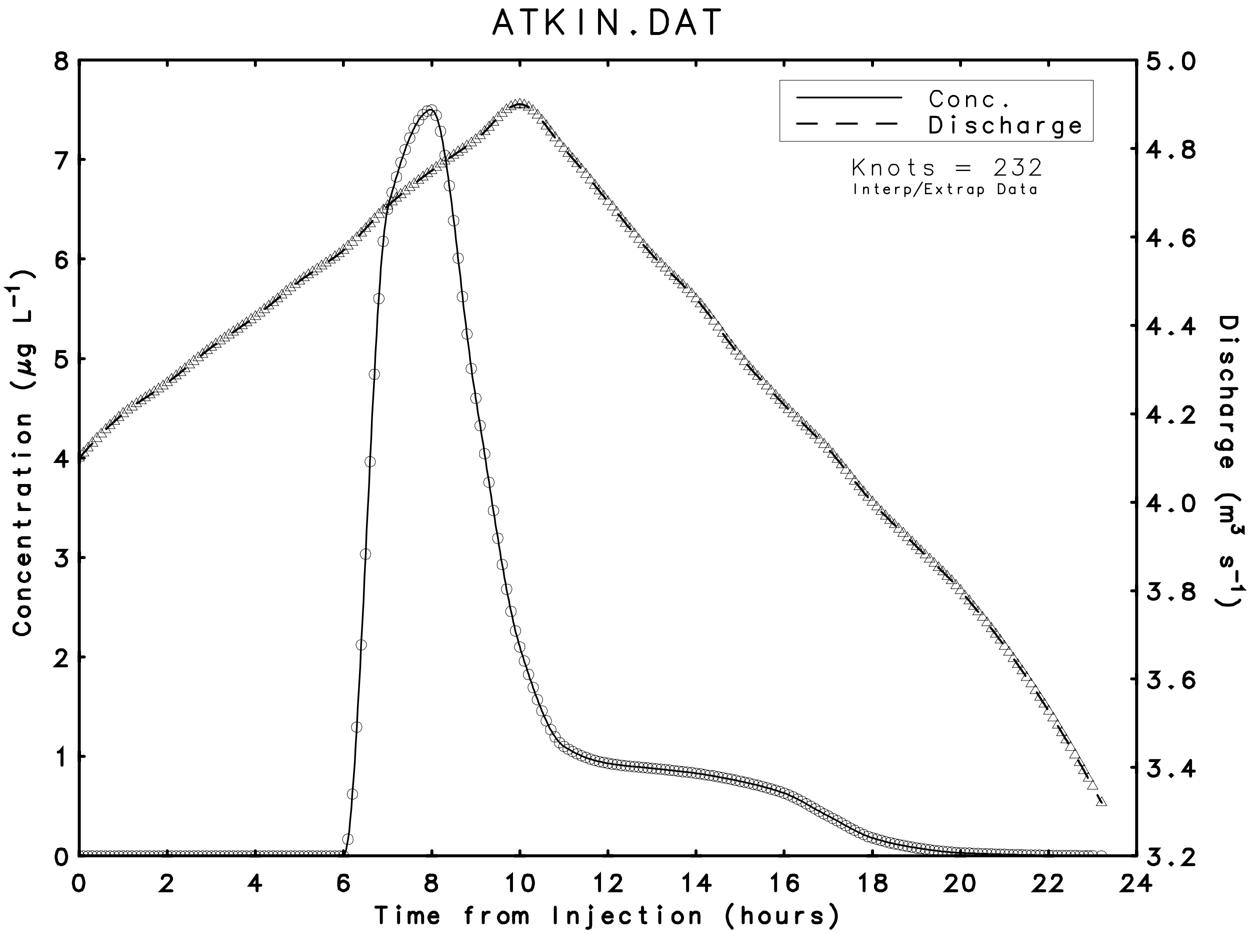

Figure 32. Interpolated and extrapolated data set for the ATKIN.DAT sampling station data file.

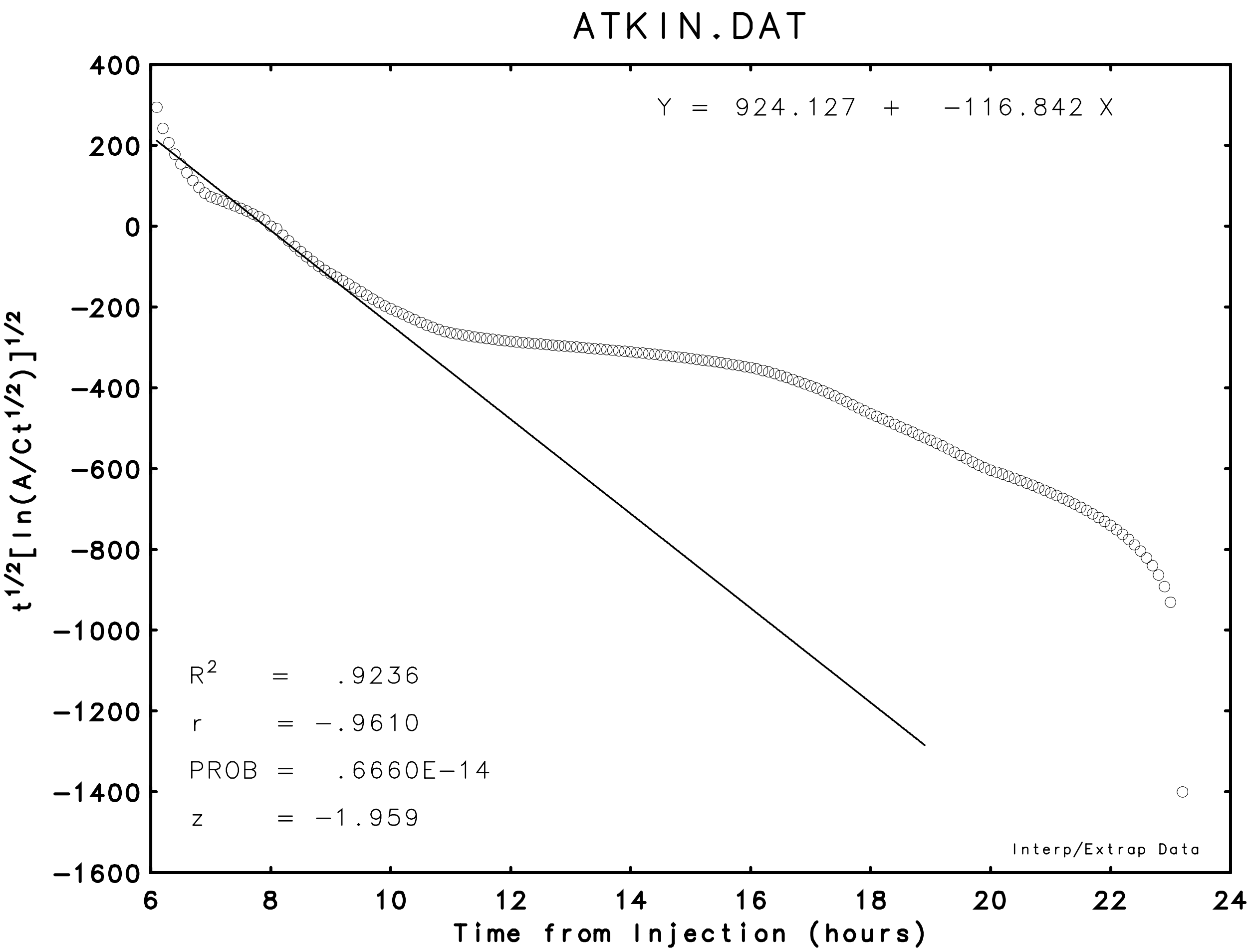

Figure 33. Interpolated and extrapolated data for the Chatwin parameter for ATKIN.DAT sampling station data file.

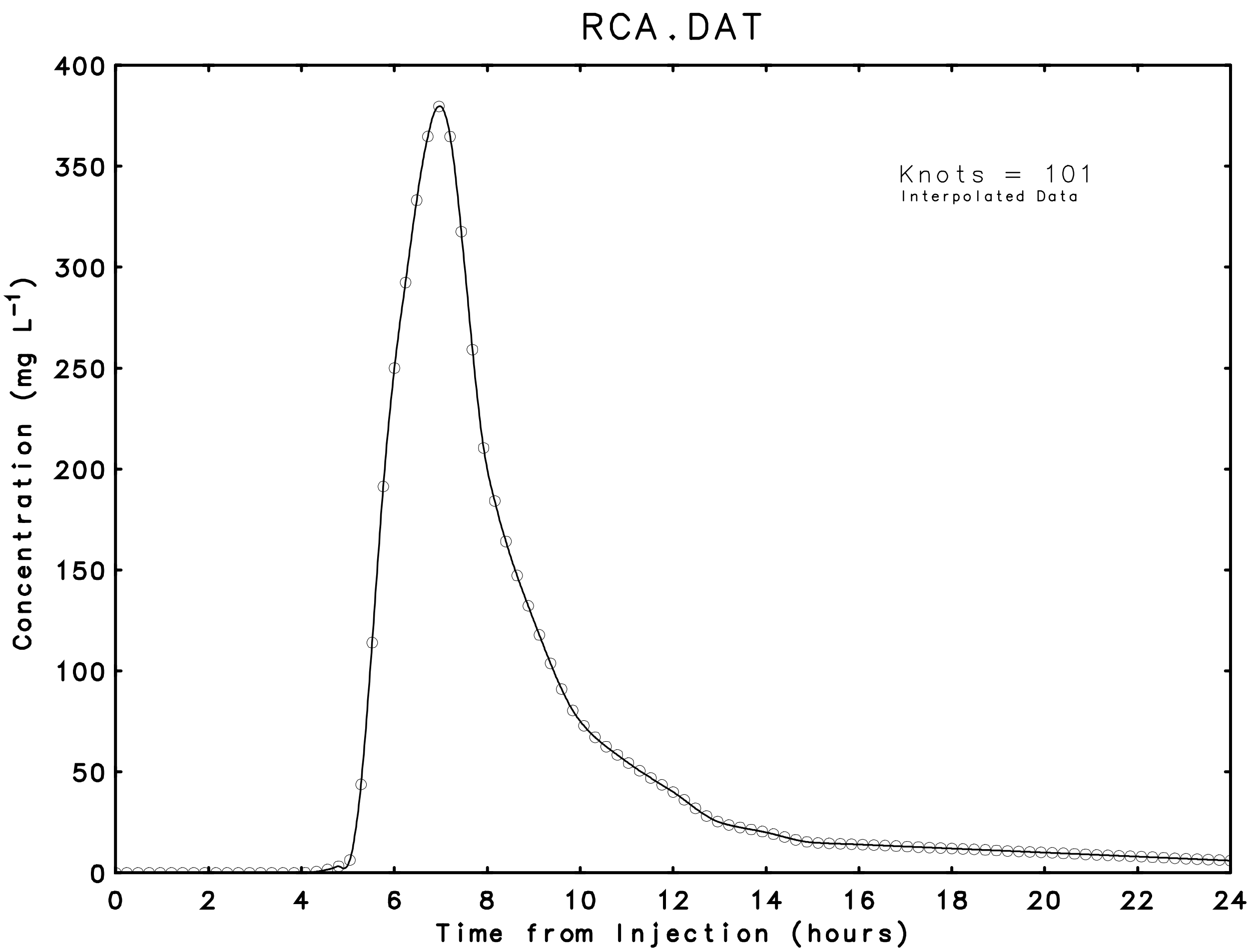

Figure 34. Interpolated curve for the RCA.DAT sampling station data file.

for the straight-line and the relevant statistics describing the straight-line fit were generated by QTRACER.

Some difference will be noted between Figure 35 and Figure 23, but not a greatly significant difference. Interpolation results in more datapoints falling on the necessary straight line, and the equation of the straight line has different values for the y intercept and slope. As such, a slightly different estimate for longitudinal dispersion will result.

Table 7 compares the final analytical output for the unaltered tracer-breakthrough curve for the RCA.DAT data set, the interpolated RCA.DAT data set, and the interpolated-extrapolated RCA.DAT data set. Note how each file's results are closely matched with the others.

8.3.3. Extrapolated RCA.DAT Tracer-Breakthrough Curve

Figure 36 depicts the extrapolated tracer-breakthrough curve generated and analyzed by QTRACER. Note that discharge has no extrapolated value because discharge was constant.

Graphically, the user will note that Figure 36 is more reasonable than Figure 22. The improvement is most evident at the elapsed time of travel. In Figure 22, the elapsed time of travel (24 hours) is reflected in a cessation of sample collection prior to "complete" tracer recovery. However, Figure 36 suggests nearly "complete" tracer recovery at > 30 hours.

8.3.4. Extrapolated RCA.DAT Chatwin Plot

Figure 37 depicts the extrapolated data plot and straight-line fit of the Chatwin parameter for longitudinal dispersion generated and analyzed by QTRACER. Note that the straight-line fit, equation for the straight-line, and relevant statistics describing the straight-line fit generated by QTRACER are slightly different from the results shown in Figure 23.

The obvious differences in between Figure 37 and Figure 23 are a result of not having continued actual data collection until near "complete" tracer recovery. Because sampling ceased before adequate tracer recovery, data extrapolation exerts considerable influence on the Chatwin analysis; in this instance, a less good straight-line fit to the data.

8.4. INTERPOLATED-EXTRAPOLATED RCA.DAT DATA

Figures 38 and 39 illustrate how the interpolation and extrapolation routines provided in QTRACER can be used in tracer-breakthrough curve analyses. Table 7 illustrates that there are no significant differences in any of the analyses provided by QTRACER for the RCA.DAT data set.

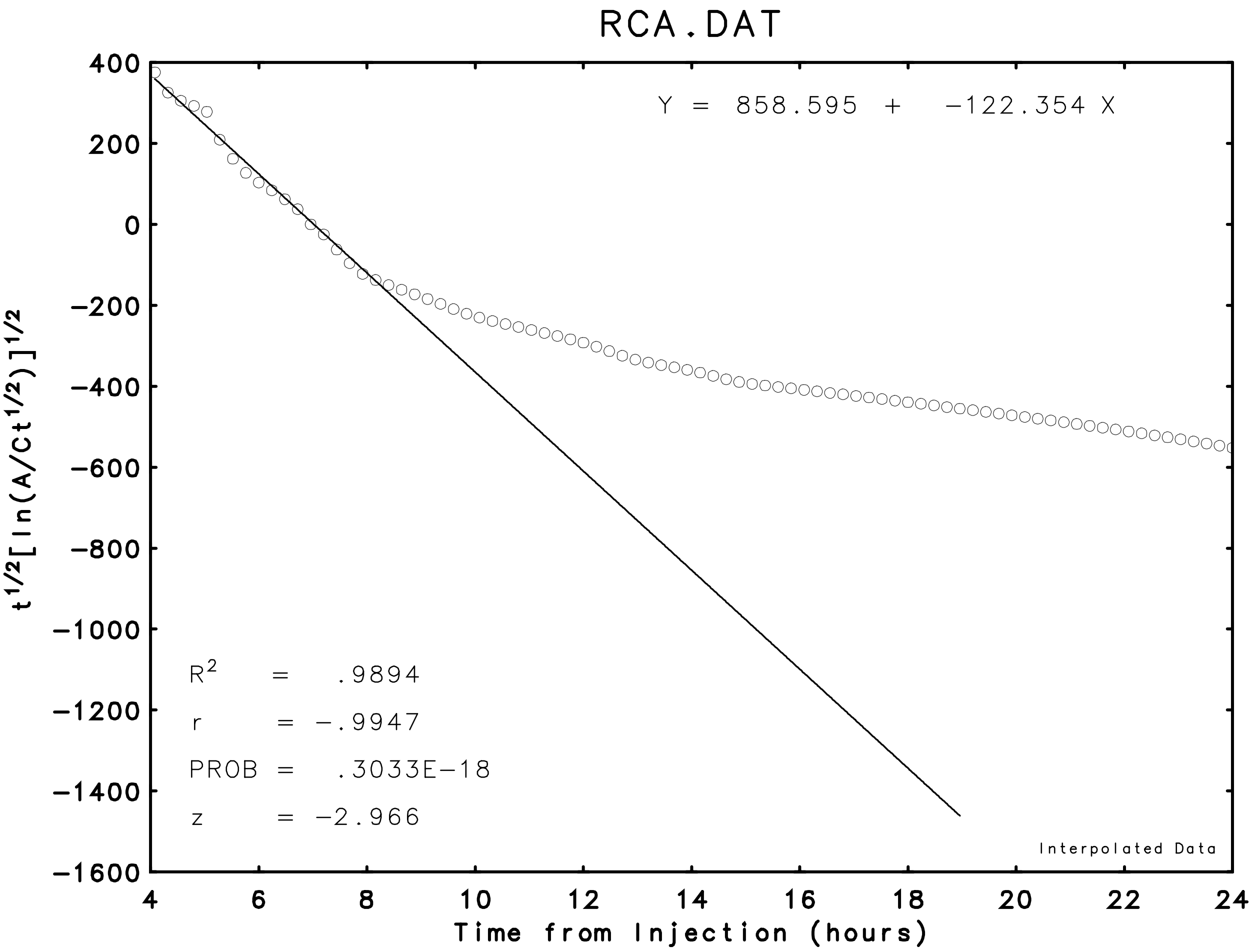

Figure 35. Interpolated data set for the Chatwin parameter for the RCA.DAT sampling station data file.

Table 7. Estimated hydraulic flow and geometric parameters from tracer-breakthrough curves for RCA.DAT sampling station.

Parameter	RCA.DAT (unaltered)	RCA.DAT (interpolated)	RCA.DAT[1] (extrapolated)	RCA.DAT[2] (inter./extra.)
Tracer Mass Recovered, g	1.74×10^{3}	1.74×10^{3}	1.77×10^{3}	1.77×10^{3}
Percent Mass Recovered	6.59×10^{-1}	6.59×10^{-1}	6.70×10^{-1}	6.71×10^{1}
Accuracy Index	9.93×10^{-1}	9.93×10^{-1}	9.93×10^{-1}	9.93×10^{-1}
Initial Tracer Breakthrough, h	5.00×10^{0}	4.08×10^{0}	5.00×10^{0}	4.08×10^{0}
Time to Peak Concentration, h	7.00×10^{0}	6.96×10^{0}	7.00×10^{0}	6.96×10^{0}
Mean Tracer Residence Time, h	8.81×10^{0}	8.80×10^{0}	9.10×10^{0}	9.15×10^{0}
Elapsed Tracer Travel Time, h	2.40×10^{1}	2.40×10^{1}	3.17×10^{1}	5.20×10^{1}
Maximum Tracer Flow Velocity, m s^{-1}	2.79×10^{-3}	3.42×10^{-3}	2.79×10^{-3}	3.42×10^{-3}
Peak Tracer Flow Velocity, m s^{-1}	2.00×10^{-3}	2.01×10^{-3}	2.00×10^{-3}	2.01×10^{-3}
Mean Tracer Flow Velocity, m s^{-1}	1.59×10^{-3}	1.59×10^{-3}	1.54×10^{-3}	1.53×10^{-3}
Shear Velocity, m s^{-1}	2.88×10^{-4}	2.88×10^{-4}	2.81×10^{-4}	2.80×10^{-4}
Longitudinal Dispersion, m^2 s^{-1}	7.19×10^{-4}	8.58×10^{-4}	9.24×10^{-4}	9.32×10^{-4}
Hydraulic Head Loss, m	9.82×10^{-7}	9.83×10^{-7}	9.20×10^{-7}	9.10×10^{-7}

Listed parameters without dimensions are dimensionless.
[1]Extrapolated using a cubic Hermite function.
[2]Extrapolated using an exponential decay function.

Table 7. Estimated hydraulic flow and geometric parameters from tracer-breakthrough curves for RCA.DAT sampling station (cont.).

Parameter	RCA.DAT (unaltered)	RCA.DAT (interpolated)	RCA.DAT[1] (extrapolated)	RCA.DAT[2] (inter./extra.)
Conduit Volume, m^3	1.20×10^{1}	1.20×10^{1}	1.24×10^{1}	1.25×10^{1}
Conduit Cross-Sectional Area, m^2	2.39×10^{-1}	2.39×10^{-1}	2.47×10^{-1}	2.48×10^{-1}
Conduit Surface Area, m^2	3.50×10^{4}	3.50×10^{4}	3.47×10^{4}	3.47×10^{4}
Tracer Sorption Coefficient, m	5.17×10^{-2}	5.16×10^{-2}	5.29×10^{-2}	5.32×10^{-2}
Conduit Diameter, m	5.51×10^{-1}	5.51×10^{-1}	5.60×10^{-1}	5.62×10^{-1}
Friction Factor	8.34×10^{-2}	8.34×10^{-2}	8.48×10^{-2}	8.50×10^{-2}
Laminar Hydraulic Conductivity, m s^{-1}	8.17×10^{4}	8.16×10^{4}	8.44×10^{4}	8.48×10^{4}
Reynolds Number	7.67×10^{2}	7.67×10^{2}	7.55×10^{2}	7.53×10^{2}
Froude Number	7.70×10^{-4}	7.71×10^{-4}	7.40×10^{-4}	7.34×10^{-4}
Peclet Number	1.40×10^{2}	1.18×10^{2}	1.09×10^{2}	1.08×10^{2}
Schmidt Number	1.14×10^{3}	1.14×10^{3}	1.14×10^{3}	1.14×10^{3}
Sherwood Number	1.22×10^{2}	1.22×10^{2}	1.22×10^{2}	1.22×10^{2}
Mass Transfer Coefficient, m s^{-1}	2.22×10^{-7}	2.22×10^{-7}	2.19×10^{-7}	2.18×10^{-2}
Molecular diffusion layer, m	4.50×10^{-3}	4.50×10^{-3}	4.58×10^{-3}	4.59×10^{-3}

Listed parameters without dimensions are dimensionless.
[1]Extrapolated using a cubic Hermite function.
[2]Extrapolated using an exponential decay function.

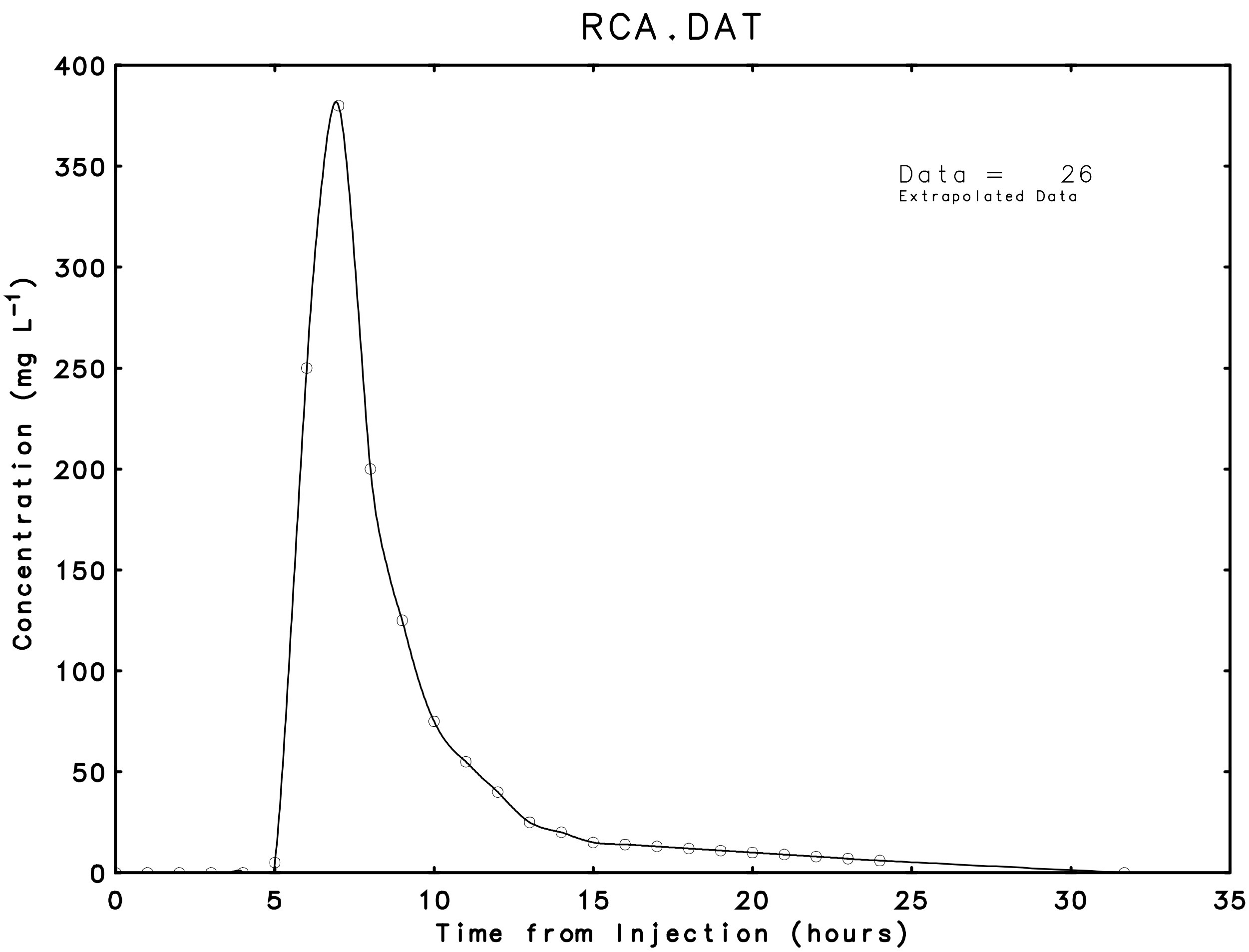

Figure 36. Extrapolated curve for the RCA.DAT sampling station data file.

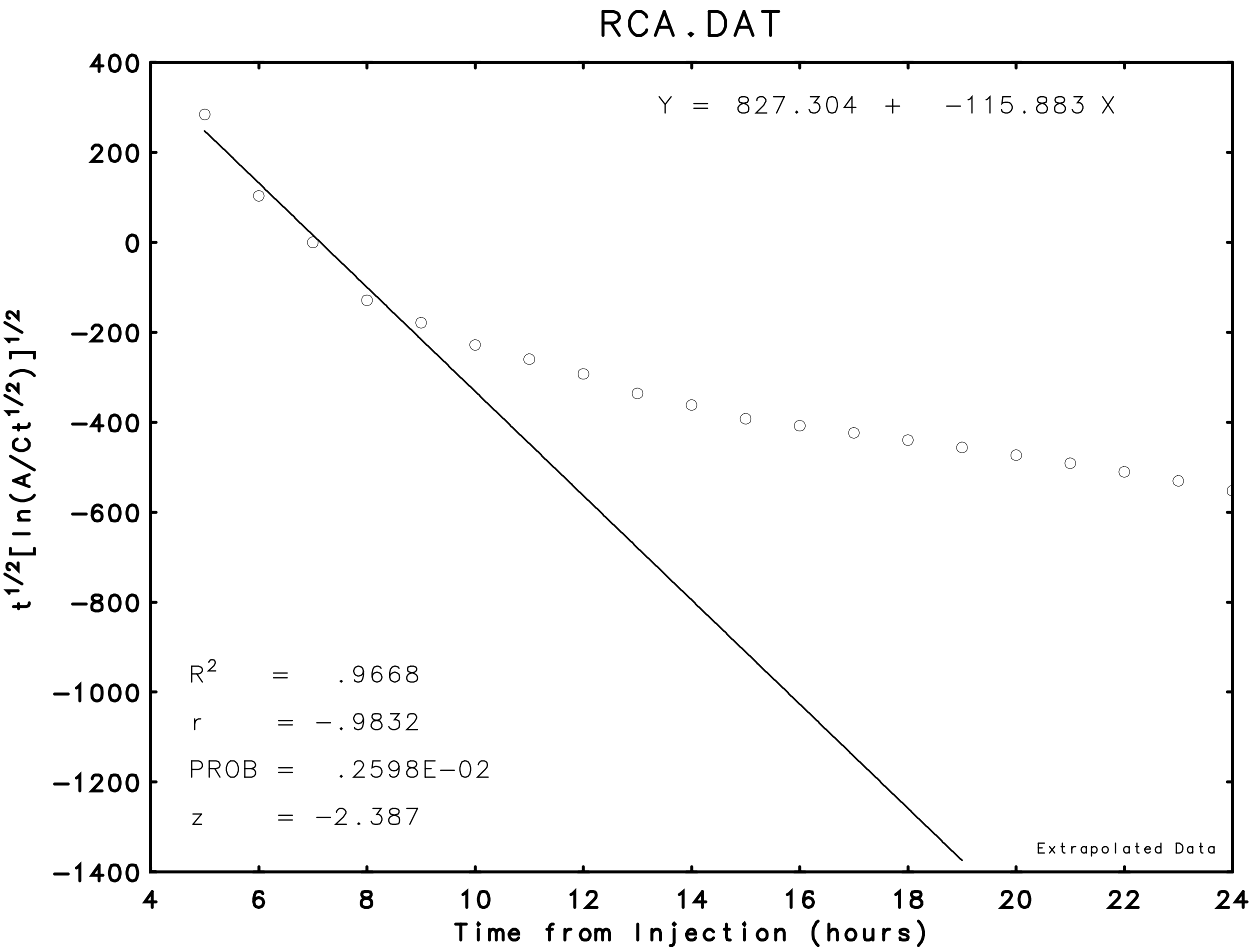

Figure 37. Extrapolated data set for the Chatwin parameter for the RCA.DAT sampling station data file.

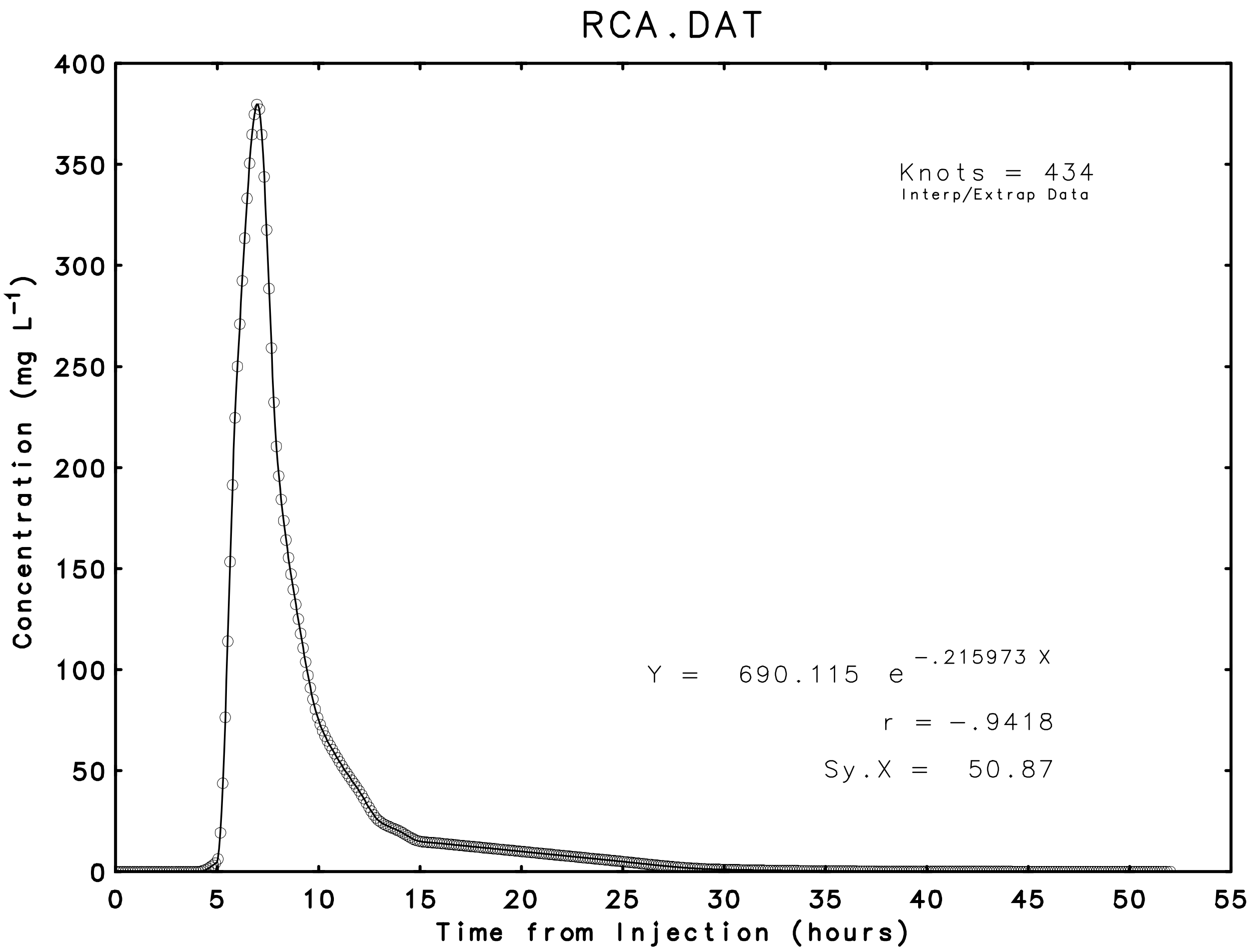

Figure 38. Interpolated and extrapolated data set for the RCA.DAT sampling station data file.

The user will note in Figures 38 that the exponential decay equation

$$y = 690.115e^{-0.21597x} \tag{50}$$

has been produced along with the correlation coefficient r (-0.9418) and the standard error of the estimated fit (50.87). QTRACER provides this information to the user to assist in assessing the effect of an exponential decay on a tracer-breakthrough curve. It will be noted that whereas extrapolation methods `2` (piecewise cubic Hermite) and `3` (statistical method) produce a single extrapolated point, method `1` (exponential decay) produces five additional datapoints and thus has a great deal more influence on the final results.

Exponential decay extrapolation has more influence because the integration routine employed by QTRACER is forced to conform to the shape of the exponentially decaying curve. It is therefore incumbent upon the user to determine the appropriateness of using an exponential decay model for extrapolation. For example, applying an exponential decay for extrapolation to the ATKIN.DAT data set results in tracer mass recovery that is greater than what was injected. Clearly this is an impossibility that suggests major field errors, laboratory errors, numerical errors, or some combination of all three.

A more erratic tracer-breakthrough curve or one that was ended leaving a significant mass of tracer in the system would result in large differences when data interpolation and/or extrapolation is employed. The user should note that when data extrapolation is employed without data interpolation, the graphics may appear incorrect (*i.e.*, a straight-line connection from the last measured datapoint to the extrapolated datapoint). This apparent inaccuracy is not a problem, however, as it is strictly an artifact of the plotting algorithm. The integration routine used by QTRACER will develop a smooth curve between all provided datapoints regardless of tracer-breakthrough curve appearance.

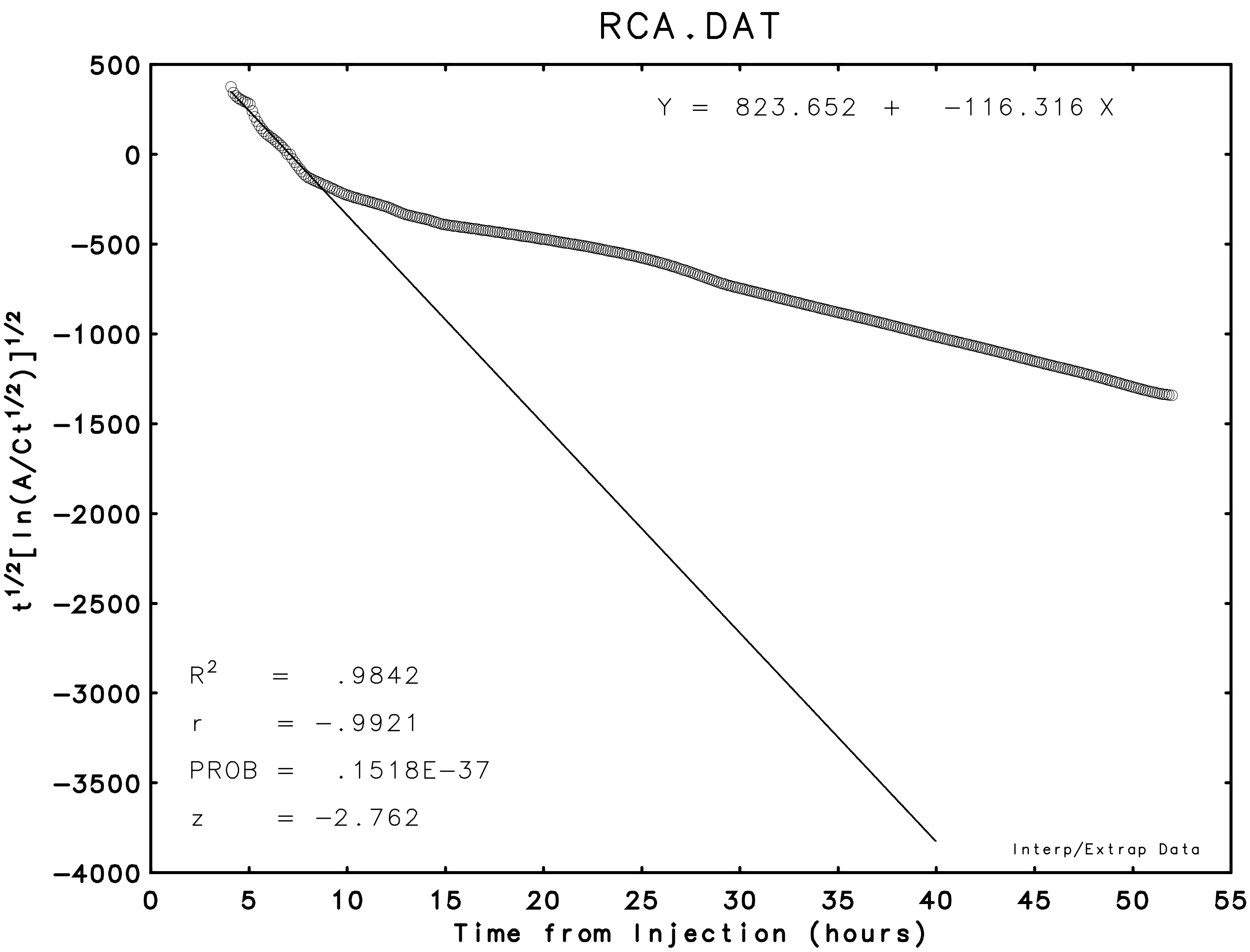

Figure 39. Interpolated and extrapolated data for the Chatwin parameter for RCA.DAT sampling station data file.